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High order adaptive methods of Nyström–Cowell type

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Abstract

A class of unconditionally stable multistep methods is discussed for solving initial-value problems of second-order differential equations which have periodic or quasiperiodic solutions. This situation frequently occurs in celestial mechanics, in nonlinear oscillations and various other situations. The methods depend upon a parameter $\omega > 0$, and integrate exactly trigonometric functions along with algebraic polynomials. In this paper we show a procedure for the construction of adaptive Nyström–Cowell formulas of arbitrarily high order of accuracy, and reduce to the classical Nyström–Cowell methods for $\omega = 0$. Our methods compare advantageously with other methods.

Keywords: Second-order initial-value problems; Adaptive Nyström–Cowell methods; Orbital unstability

AMS classification: 65L05; 65L20

1. Introduction

In this paper we present new methods, which we call adaptive Nyström–Cowell methods, for the numerical integration of second-order initial-value problems of the form

$$\begin{aligned} &\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + \omega^2 y = f(t, y), \quad 0 < t \leqslant T, \quad \omega > 0, \quad y \in \mathbb{R}^n, \\ &y(0) = y_0, \qquad y'(0) = y_0', \end{aligned} \tag{1.1}$$

where the main frequency ω may be known or accurately estimated and the perturbing force $f(t, y)$ is assumed to be small relative to the force $\omega^2 y$, i.e. $f(t, y) = \varepsilon g(t, y)$, ε being a small parameter ($\varepsilon \ll 1$). These methods are designed in such a way that, for the unperturbed problem $f(t, y) = 0$, the error of the free oscillations in the numerical solution is null. In other words, the methods presented

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integrate exactly the unperturbed problem. Methods having this property are suitable for long interval integration of perturbed systems of type (1.1), because the integration step size may be chosen much larger than the step size needed for classical multistep methods. Besides, the numerical deficiency known as *orbital unstability* (see [11]) is avoided.

In several previous papers, [4, 9], we have introduced and studied a class of adaptive Störmer–Cowell methods. The adaptive Nyström–Cowell methods are different from the adaptive Störmer–Cowell methods by the way they choose the coefficients at each step of the integration. The new selection is meant to improve the efficiency of the adaptive Störmer–Cowell methods and the other classical multistep methods. That they do so, we shall show in Section 4.

In order to integrate the initial-value problem (1.1), it is desirable to use methods that do not require introducing the derivatives y' since they are not explicitly contained in the perturbation force. Assuming the main frequency of oscillation is a priori known (exactly or to a good approximation), a kind of adaptive Störmer–Cowell formula for the numerical integration of Eq. (1.1) has the form [9].

$$\sum_{j=0}^{k} \alpha_j(v) y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j(v) f(t_{n+j}, y_{n+j}), \qquad v = \omega h, \tag{1.2}$$

where the coefficients $\alpha_j(v)$ and $\beta_j(v)$ are assumed to be continuous functions for each $v \in [0, \Lambda]$, for an $\Lambda > 0$ given. The development of the integration procedure (1.2) follows the idea given in Correas (1977, 1978) and it is characterized by the linear truncation error operators L_h, defined as follows:

$$L_h[y(t)] = \sum_{i=0}^{k} [\alpha_j(v) y(t+jh) - h^2 \beta_j(v)\{y''(t+jh) + \omega^2 y(t+jh)\}]. \tag{1.3}$$

Furthermore, Correas imposes that the kernel of L_h contain the linear spaces $\Pi_p(\omega)$ generated by the modified Stumpff functions $\phi_i(t, \omega)$, $i = 0, 1, \ldots, p$, where

$$\phi_0(t, \omega) = \begin{cases} \cos \omega t & \text{if } \omega \neq 0, \\ 1 & \text{if } \omega = 0, \end{cases}$$

$$\phi_{i+1}(t, \omega) = \int_0^t \phi_i(t, \omega)\, \mathrm{d}t, \quad i \geqslant 0.$$

The linear space $\Pi_p(\omega)$ generated by the functions $\phi_i(t, \omega)$ may be expressed in the form

$$\Pi_p(\omega) = \begin{cases} \mathrm{Span}\{1, t, t^2, \ldots, t^{p-2}, \cos \omega t, \sin \omega t\} & \text{if } \omega \neq 0, \\ \mathrm{Span}\{1, t, t^2, \ldots, t^{p-2}, t^{p-1}, t^p\} & \text{if } \omega = 0. \end{cases}$$

Consequently, if $\omega = 0$, the difference equations (1.2) reduces to the classical multistep methods with constant coefficients.

The connection between spaces $\Pi_p(\omega)$, the linear operators L_h and the order of consistency of the methods are as follows [9].

Order conditions: The linear operator L_h associated with the adaptive method (1.2) annihilates the space $\Pi_{p+1}(\omega)$ if and only if the following conditions are verified:

$$\begin{aligned}
D_0 &= \sum_{j=0}^{k} \alpha_j(v)\phi_0(j, v) = 0,\\
D_1 &= \sum_{j=0}^{k} \alpha_j(v)\phi_1(j, v) = 0, \qquad (1.4)\\
D_i &= \sum_{j=0}^{k} [\{\alpha_j(v) - v^2\beta_j(v)\}\phi_i(j, v) - \beta_j(v)\phi_{i-2}(j, v)] = 0, \quad i = 2, 3, \ldots, p+1.
\end{aligned}$$

Besides, these conditions are sufficient at order p for all ω real. The necessary and sufficient conditions are

$$D_0 = 0(h^{p+2}), \qquad D_1 = 0(h^{p+1}), \ldots, D_{p+1} = 0(h). \qquad (1.5)$$

Under the hypothesis of consistency of order one and the following roots condition

If $\zeta(v)$ is a root of $\rho(\zeta, v)$, there exists a positive constant C such that $|\zeta(v)| \leqslant \exp(Cv)$. Besides, if $\zeta(v)$ is a root of $\rho(\zeta, v)$ with multiplicity greater than two, then $|\zeta(v)| < 1$ for all $v \in [0, \Lambda]$,

the method (1.2) is convergent (see [4, 9]).

Definition. We call the method (1.2) an adaptive Nyström–Cowell (adaptive-NC) method if

$$\alpha_k(v) = 1, \qquad \alpha_{k-2}(v) = -2\phi_0(2, v), \qquad \alpha_{k-4}(v) = 1,$$
$$\alpha_j(v) = 0, \quad j \neq k, k-2, k-4,$$

To distinguish them from the methods characterized by the conditions

$$\alpha_k(v) = 1, \qquad \alpha_{k-1}(v) = -2\phi_0(1, v), \qquad \alpha_{k-2}(v) = 1,$$
$$\alpha_j(v) = 0, \quad j \neq k, k-1, k-2,$$

we shall call the latter the adaptive Störmer–Cowell (adaptive-SC) methods.

In Section 2, we construct an accurate and efficient procedure for the integration of dynamical systems of type (1.1), These algorithms are built for arbitrarily high order of accuracy; they are very easy to implement in a digital computer. Besides, we prove that the local truncation error constants of the adaptive-NC methods are smaller than that corresponding to the adaptive-SC methods. This feature was already known (see [5]) for the classical methods of constant coefficients ($v = 0$). In Section 3, the stability of the adaptive methods is discussed using the standard linear test model. In Section 4, we compare numerically these methods to adaptive Störmer–Cowell methods [4, 9] and other classical ones. We conclude with a few results from the numerical experiments realized.

2. Derivation of the adaptive Nyström–Cowell methods

One may think of constructing adaptive methods by solving the linear system given by conditions (1.4). The process, however, is unsuitable in practice for methods of a high order. As an example of the complexity one would encounter, see the paper of Neta and Ford [8]. One overcomes the difficulty by means of recurrent algorithms for a class of adaptive methods, namely the Nyström–Cowell methods.

To this effect, the general solution of problem (1.1) can be written as

$$y(t) = C_1\phi_0(t,\omega) + C_2\phi_1(t,\omega) + \int_{t_n}^{t} f(s)\phi_1(t-s,\omega)\,\mathrm{d}s, \tag{2.1}$$

where C_1 and C_2 are arbitrary constants, ω is the main frequency of problem (1.1). By an abuse of notation, we write $f(s)$ to designate $f(s, y(s))$. Substituting t_{n+i}, t_n and t_{n-i} for t in (2.1) and eliminating C_1 and C_2 from the resulting equations, we obtain

$$y(t_{n+i}) - 2\phi_0(i,v)y(t_n) + y(t_{n-i}) = \int_{t_n}^{t_{n+i}} [f(s) + f(2t_n - s)]\,\phi_1(t_{n+i}-s,\omega)\,\mathrm{d}s,$$

with $v = \omega h$. This equation is obtained for the case $i = 1$ in [4], and it is used for the construction of adaptive-SC methods. In this section, we study the case $i = 2$ to build high-order adaptive-NC methods. Substituting the perturbing function $f(t, y)$ by the Newton backward difference interpolation polynomial in a mesh of equally spaced points $t_j = t_0 + jh$, $(0 \leqslant j \leqslant k)$, we obtain the following adaptive multistep method

$$y_{n+2} - 2\phi_0(2,v)y_n + y_{n-2} = h^2 \sum_{j=0}^{k} \sigma_{j,r}(v)\,\nabla^j f_{n+r}, \quad r = 1, 2, \tag{2.2}$$

where $r = 1$ in the explicit case, and $r = 2$ in the implicit one. In (2.2) $\nabla^j f_k$ is the jth backward difference and $f_k = f(t_k, y_k)$. The coefficient $\sigma_{j,r}(v)$ are given by the quadratures:
for the explicit case

$$\sigma_{j,1}(v) = (-1)^j \int_{-1}^{1} \left[\binom{-\tau}{j} + \binom{\tau+2}{j}\right] \phi_1(1-\tau, v)\,\mathrm{d}\tau, \tag{2.3a}$$

for the implicit case

$$\sigma_{j,2}(v) = (-1)^j \int_{-2}^{0} \left[\binom{-\tau}{j} + \binom{\tau+4}{j}\right] \phi_1(-\tau, v)\,\mathrm{d}\tau. \tag{2.3b}$$

These coefficients can be computed in a simple and recurrent form, thereby producing analytic functions $G_r(t, v)$ (generating functions); in this manner, the coefficients $\sigma_{j,r}(v)$ are precisely the coefficients of $G_r(t, v)$ expanded as a Taylor series at $t = 0$ [5].

Consider the generating functions of the form

$$G_r(t,v) = \sum_{j=0}^{\infty} \sigma_{j,r}(v)t^j, \quad r = 1, 2.$$

Substituting the values (2.3) of the coefficients $\sigma_{j,r}(v)$ and integrating by parts, we obtain the following generating functions:

$$G_r(t,v) = \frac{2(1-\phi_0(2,v))(1-t)^2 + 4t^2 - 4t^3 - t^4}{[(r-1) + (2-r)(1-t)][(\log(1-t))^2 + v^2]}, \quad r = 1, 2. \tag{2.4}$$

Note that, when the parameter v tends to zero, the generating functions (2.4) tend to

$$G_1(t,0)=\frac{4t^2-4t^3-t^4}{(1-t)(\log(1-t))^2},\quad G_2(t,0)=\frac{4t^2-4t^3-t^4}{(\log(1-t))^2},$$

and therefore coincide with the generating functions obtained in [5] for the classical Nyström–Cowell methods.

Considering the Taylor's developments of the functions appearing in the generating functions (2.4) at $t=0$, the coefficients $\sigma_{j,r}(v)$ may be obtained in a recurrent way
for the explicit case:

$$\sigma_{0,1}=\frac{1}{v^2}[2(1-\phi_0(2,v))],\quad \sigma_{1,1}=-\sigma_{0,1},$$

$$\sigma_{2,1}=\frac{1}{v^2}[4-\sigma_{0,1}],\quad \sigma_{3,1}=0,$$

$$\sigma_{n+2,1}=\frac{1}{v^2}\left[1-\sigma_{n,1}-\frac{2}{3}h_2\sigma_{n-1,1}-\frac{2}{4}h_3\sigma_{n-2,1}-\cdots-\frac{2}{n+2}h_{n+1}\sigma_{0,1}\right],\quad n\geqslant 2,$$

for implicit case:

$$\sigma_{0,2}=\frac{1}{v^2}[2(1-\phi_0(2,v))],\qquad \sigma_{1,2}=-2\sigma_{0,2},\qquad \sigma_{2,2}=\frac{1}{v^2}[4+2(1-\phi_0(2,v))-\sigma_{0,2}],$$

$$\sigma_{3,2}=-\frac{1}{v^2}[4+\sigma_{0,2}+\sigma_{1,2}],\qquad \sigma_{4,2}=\frac{1}{v^2}[(1-11/12\sigma_{0,2}-\sigma_{1,2}-\sigma_{2,2}],$$

$$\sigma_{n+2,2}=\frac{1}{v^2}\left[-\sigma_{n,2}-\frac{2}{3}h_2\sigma_{n-1,2}-\frac{2}{4}h_3\sigma_{n-2,2}-\cdots-\frac{2}{n+2}h_{n+1}\sigma_{0,2}\right],\quad n\geqslant 3,$$

where $h_n=1+\frac{1}{2}+\cdots+1/n$.

In this situation, we may write the method (2.2) in Lagrangian form as

For $r=1,2$

$$y_{n+2}-2\phi_0(2,v)y_n+y_{n-2}=h^2\sum_{j=0}^{k}\beta_{j,r}(v)f_{n+r-j}, \tag{2.5}$$

with coefficients

$$\beta_{j,r}(v)=(-1)^j\sum_{s=0}^{k-j}\binom{j+s}{j}\sigma_{j+s,r}(v).$$

The above recurrence relations makes the construction of adaptive methods up to any order quite easy.

2.1. First-derivative determination

When it is needed to calculate the first derivative y' or when y' appears in the perturbing force, we shall use a procedure nearly identical to that presented above. We begin by differentiating (2.1) to obtain

$$y'(t) = -\omega^2 C_1 \phi_1(t,\omega) + C_2\phi_0(t,\omega) + \int_{t_n}^{t} f(s)\phi_0(t-s,\omega)\,\mathrm{d}s. \tag{2.6}$$

Following the same way as for the solution $y(t)$, we obtain the scheme in differences

For $r = 1, 2$

$$y'_{n+2} - 2\phi_0(2,\nu)y'_n + y'_{n-2} = h\sum_{j=0}^{k} \sigma'_{j,r}(\nu)\, \nabla^j f_{n+r}. \tag{2.7}$$

There the coefficients $\sigma'_{j,r}(\nu)$ are found from the generating function,

$$G'_r(t,\nu) = -\frac{2(1-\phi_0(2,\nu))(1-t)^2 + 4t^2 - 4t^3 - t^4}{[(r-1)+(2-r)(1-t)][(\log(1-t))^2+\nu^2]}\log(1-t), \quad r = 1, 2, \tag{2.8}$$

and are given by the following recursive expressions:
in the explicit case:

$$\sigma'_{0,1} = 0, \qquad \sigma'_{1,1} = \frac{1}{\nu^2}[2(1-\phi_0(2,\nu))], \qquad \sigma'_{2,1} = -\sigma'_{1,1}/2,$$

$$\sigma'_{3,1} = \frac{1}{\nu^2}[4 - (1-\phi_0(2,\nu))/3 - \sigma'_{1,1}], \qquad \sigma'_{4,1} = \sigma'_{3,1}/2,$$

$$\sigma'_{n+2,1} = \frac{1}{\nu^2}\left[\frac{4}{n} + h_{n-2} - \frac{2(1-\phi_0(2,\nu))}{(n+2)(n+1)} - \sigma'_{n,1} - \frac{2}{3}\,h_2\sigma'_{n-1,1}\right.$$
$$\left. - \frac{2}{4}h_3\sigma'_{n-2,1} - \cdots - \frac{2}{n+2}h_{n+1}\sigma'_{0,1}\right], \quad n \geqslant 3;$$

in the implicit case:

$$\sigma'_{0,2} = 0, \qquad \sigma'_{1,2} = \frac{1}{\nu^2}[2(1-\phi_0(2,\nu))], \qquad \sigma'_{2,2} = -\sigma'_{1,2}/3,$$

$$\sigma'_{3,2} = \frac{1}{\nu^2}[4 + 2(1-\phi_0(2,\nu))/3 - \sigma'_{1,2}], \qquad \sigma'_{4,2} = \frac{1}{\nu^2}[(1-\phi_0(2,\nu))/6 - 2 + \sigma'_{1,2}/2],$$

$$\sigma'_{n+2,2} = \frac{1}{\nu^2}\left[\frac{4}{n} - \frac{4}{n-1} + \frac{1}{n-2} + \frac{4(1-\phi_0(2,\nu))}{(n+2)(n+1)n} - \sigma'_{n,2}\right.$$
$$\left. - \frac{2}{3}\,h_2\sigma'_{n-1,2} - \frac{2}{4}h_3\sigma'_{n-2,2} - \cdots - \frac{2}{n+2}h_{n+1}\sigma'_{0,2}\right], \quad n \geqslant 3,$$

where $h_n = 1 + \frac{1}{2} + \cdots + 1/n$.

Now we shall compare the local truncation error constants of the methods obtained here, with the adaptive-SC methods obtained in [4], including even the constant coefficient case ($v = 0$).

With a suitable choice of i and s, the adaptive-SC and adaptive-NC methods can be brought into the form

$$y_{n+i} - 2\phi_0(i, v) y_n + y_{n-i} = h^2 \sum_{j=0}^{k} \sigma_j(v)\, \nabla^j f_{n+s}. \tag{2.9}$$

Assuming that function $y(t)$ has derivatives of sufficiently high order, the local truncation error operator can be expressed by

$$L_h[y(t)] = y(t_{n+i}) - 2\phi_0(i, v) y(t_n) + y(t_{n-i}) - h^2 \sum_{j=0}^{k} \sigma_j(v)\, \nabla^j \{y''(t_{n+s}) + \omega^2 y(t_{n+s})\}.$$

After some algebra and using the mean-value theorem of the integral calculus we obtain

$$L_h[y(t)] = h^{k+3} \sigma_{k+1}(v) \{y^{(k+3)}(\zeta) + \omega^2 y^{(k+1)}(\zeta)\}, \quad t_{n+s-k} < \zeta < t_{n+s}. \tag{2.10}$$

Therefore, following Henrici [5], if $\sigma_{k+1}(v) \neq 0$, the error constant is given by

$$C_k(v) = \sigma_{k+1}(v)/\sigma_0(v),$$

and the resulting k-step method has order $k + 1$.

In the appendix we present the local truncation error constants for the implicit adaptive-NC and adaptive-SC methods (thereafter they will be used for numerical comparisons) with the number of steps $k = 4, 5, 6, 7, 8$. We denote by $C_k^N(v)$ the error constant of the local truncation error operator for the k-step adaptive-NC method and by $C_k^S(v)$ the same for the k-step adaptive-SC method. As it was expected, when $v = 0$ the constant coincides with the one of the constant coefficient methods. We also present some figures where we draw the absolute value of the ratio between the error constants corresponding, respectively, to the adaptive-NC and adaptive-SC methods $|C_k^N(v)/C_k^S(v)|$ for $v \in [0, 2]$. From these pictures one realizes that the constants $C_k^N(v)$ are of a smaller size than the constants $C_k^S(v)$. This fact was already known for the classical methods of constant coefficients and, as we shall see in Section 4, it will imply an improvement of the numerical results of the adaptive-NC methods against the adaptive-SC methods.

3. Linear stability of the methods

In this section, we study the stability of the adaptive methods when they are applied to the standard linear test method.

Definition. A multistep method, when it is applied to the linear test model $y'' + \lambda^2 y = 0$, is said to be *unconditionally stable* if all the roots $\zeta_j(H)$ of the stability polynomial (characteristic polynomial) satisfy the condition

$$|\zeta_j(H)| \leqslant 1 \quad \text{for all } H = \lambda h > 0, \tag{3.1}$$

and the multiple roots are $|\zeta_j(H)| < 1$. When condition (3.1) is satisfied for all $H \in (0, \gamma)$, this interval is called the *stability interval* of the method.

Let us test the adaptive methods with the standard linear test model as given in the form

$$y'' + \omega^2 y = -\varepsilon y, \tag{3.2}$$

where $\varepsilon = \lambda^2 - \omega^2$ and indicates the type of approximation for which the main frequency of the problem, λ, is estimated by the parameter ω. If the method (2.5) is used to solve Eq. (3.2), the numerical solution satisfies the difference equation

$$y_{n+2} - 2(\cos 2v) y_n + y_{n-2} = -h^2 \varepsilon \sum_{j=0}^{k} \beta_j(v) y_{n+r-j}. \tag{3.3}$$

Denoting $z = \varepsilon h^2$, the characteristics equation associated with the difference Eq. (3.3) can be expressed in the form

$$z = -\zeta^{k-2}(\zeta^2 - 2\cos 2v + \zeta^{-2}) / \textstyle\sum_{j=0}^{k} \beta_j(v) \zeta^{k-j}. \tag{3.4}$$

In order that z to take values such that the roots of (3.4) lie on the unit circle, we put $\zeta(v) = e^{i\theta}$, $0 \leqslant \theta \leqslant 2\pi$ into (3.4) and, after simplifications, we obtain

$$z(\theta) = \frac{2(\cos 2v - \cos 2\theta)}{R^2 + S^2} \begin{cases} R\cos(k-2)\theta + S\sin(k-2)\theta, \\ + i(R\sin(k-2)\theta - S\cos(k-2)\theta), \end{cases} \tag{3.5}$$

where the quantities R and S represent the Fourier sums

$$R = \beta_0(v)\cos k\theta + \beta_1(v)\cos(k-1)\theta + \cdots + \beta_k(v),$$

$$S = \beta_0(v)\sin k\theta + \beta_1(v)\sin(k-1)\theta + \cdots + \beta_{k-1}(v)\sin\theta.$$

Expression (3.5) provides the equations that define the boundary of the stability region in the complex plane (boundary locus) for the adaptive-NC methods.

In a similar way, the characteristic equation and the boundary locus for the adaptive-SC methods are given, respectively, by

$$z = -\zeta^{k-2}(\zeta^2 - 2(\cos v)\zeta + 1) / \textstyle\sum_{j=0}^{k} \beta_j(v) \zeta^{k-j}, \tag{3.6}$$

$$z(\theta) = \frac{2(\cos v - \cos\theta)}{R^2 + S^2} \begin{cases} R\cos(k-1)\theta + S\sin(k-1)\theta \\ + i(R\sin(k-1)\theta - S\cos(k-1)\theta). \end{cases} \tag{3.7}$$

Now we analyze the properties concerning the stability of the adaptive methods for those cases of practical interest.

3.1. The main frequency of the problem is exactly known

This occurs when the main frequency λ is exactly equal to parameter ω, and then $\varepsilon = 0$. In this case $z = 0$, and the stability polynomial (3.4) for the adaptive-NC methods reduces to

$$(\zeta^4 - 2(\cos 2v)\zeta^2 + 1)\zeta^{k-4} = 0, \tag{3.8}$$

so that the roots are $\zeta_1(v) = e^{iv}$, $\zeta_2(v) = -e^{iv}$, $\zeta_3(v) = e^{-iv}$, $\zeta_4(v) = -e^{-iv}$, $\zeta_j(v) = 0, j \geqslant 5$. In other words, the principal roots are simple and they are on the unit circle. Besides, the spurious roots are null.

Similarly, the stability polynomial (3.6) for the adaptive-SC methods reduces to

$$(\zeta^2 - 2(\cos v)\zeta + 1)\zeta^{k-2} = 0, \tag{3.9}$$

so that the roots are $\zeta_1(v) = e^{iv}$, $\zeta_2(v) = e^{-iv}$, $\zeta_j(v) = 0$, $j \geqslant 3$. We may thus conclude that the adaptive-NC and adaptive-SC methods, in this case, are both *unconditionally stable.*

3.2. The main frequency of the problem is not exactly known

This occurs when the main frequency λ is only estimated by the parameter ω, and so $\varepsilon \neq 0$. In this case, the adaptive schemes result to be conditionally stable. We have calculated numerically the stability intervals for the implicit adaptive-SC and adaptive-NC methods with $k = 4, 5, 6, 7, 8$ and different values of the parameter v. These intervals are presented in Tables 1, 2 (the stars "******" meaning that the length of the interval is smaller than 0.01), and when $v = 0$ they correspond to the stability intervals associated with the classical methods of constant coefficients.

It is easily noticed that for the classical-NC methods of constant coefficients ($v = 0$), the stability intervals are empty. For this reason their use has not been extended and in the literature they have not received much attention when compared with other methods. On the contrary, if $v \neq 0$, it may be observed that the stability interval of the methods is nonempty (see Table 2). Hence, the methods

Table 1
Stability intervals for the adaptive Störmer–Cowell methods

	$k=4$	$k=5$	$k=6$	$k=7$	$k=8$
$v=0$	(0, 5.45)	(0, 4.61)	(0, 3.63)	(0, 0.21)	(0, 0.40)
$v=0.1$	(0, 5.44)	(0, 4.60)	(0, 3.62)	(0, 0.20)	(0, 0.38)
$v=0.2$	(0, 5.42)	(0, 4.58)	(0, 3.61)	(0, 0.17)	(0, 0.36)
$v=0.3$	(0, 5.38)	(0, 4.55)	(0, 3.58)	(0, 0.14)	(0, 0.31)
$v=0.5$	(0, 5.25)	(0, 4.43)	(0, 3.48)	(0, 0.05)	(0, 0.18)
$v=0.7$	(0, 5.06)	(0, 4.26)	(0, 3.34)	*******	(0, 0.03)
$v=0.9$	(0, 4.81)	(0, 4.03)	(0, 3.15)	*******	*******

Table 2
Stability intervals for the adaptive Nyström–Cowell methods

	$k=4$	$k=5$	$k=6$	$k=7$	$k=8$
$v=0$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$
$v=0.1$	(0, 0.14)	(0, 0.14)	(0, 0.09)	(0, 0.10)	(0, 0.03)
$v=0.2$	(0, 0.54)	(0, 0.54)	(0, 0.21)	(0, 0.22)	(0, 0.13)
$v=0.3$	(0, 1.09)	(0, 1.09)	(0, 0.18)	(0, 0.25)	(0, 0.28)
$v=0.5$	(0, 2.26)	(0, 2.26)	(0, 0.08)	(0, 0.13)	(0, 0.68)
$v=0.7$	(0, 3.14)	(0, 3.14)	(0, 0.02)	(0, 0.03)	(0, 0.48)
$v=0.9$	(0, 3.66)	(0, 3.66)	*******	*******	(0, 0.17)

we are proposing in this paper can be considered as a stabilization of the classical Nyström–Cowell methods that appeared in [5].

On the other hand, it is worth noting that, for $k = 4, 5, 6$, the stability interval of the adaptive-NC methods is smaller than the one of the adaptive-SC methods. But this does not mean a limitation for these methods after assuming that the problems to be solved are nonstiff and that the parameter ω is a good approximation of the main frequency $\lambda(\varepsilon \ll 1)$. Thus, the intervals we have obtained are adequate for preserving the stability of most of the real applications. For example, in the figures of Section 4, a good qualitative behaviour of the adaptive-NC methods can be observed, even for integration steps relatively long.

4. Numerical results

To illustrate the behaviour of the methods derived in Section 2, some numerical applications for a family of test problems are shown in the following. We consider:

(i) The present methods given by (2.5) and (2.7).
(ii) Adaptive Störmer–Cowell methods [4].
(iii) Cowell's method [5].
(iv) Adam's method [5].

using various step sizes. These methods are of multistep type and can be obtained for arbitrary high order of approximation in recurrent form. We consider all the methods with order six, that is to say, they are comparable in terms of local approximation and computational cost. The methods are implemented in predictor–corrector form (PECE) and the initialization values are computed using an eighth-order Runge–Kutta method derived by Prince and Dormand [10] with step size $h/4$, h being the step size used by the methods (i)–(iv).

Example 1. The quasi-periodic linear problem

$$z'' + \omega^2 z = \varepsilon\omega^2 \exp(\mathrm{i}\omega t), \quad t \in [0, 1000], \quad z \in \mathbb{C}$$
$$z(0) = 1, \qquad z'(0) = \mathrm{i}(\omega - \varepsilon/2).$$

Its analytic solution is given by

$$z(t) = \left(\cos \omega t + \frac{\varepsilon}{2} t \sin \omega t\right) + i\left(\sin \omega t - \frac{\varepsilon}{2} t \cos \omega t\right),$$

and it represents a perturbed circular motion on the complex plane. The numerical results have been computed for $t = 1000$ with three different integration steps, $h = \frac{1}{20}, \frac{1}{10}, \frac{1}{5}$, and, for each h, taking in turn $\omega = 1, 2, 3$. In each run we set $\varepsilon = 0.001$. The absolute errors are computed in the form $|z(t_n) - z_n|$ and they are given in Table 3.

Example 2. The nonlinear problem (*Duffing's equation*)

$$\frac{\mathrm{d}^2 u}{\mathrm{d}t^2} + (\omega^2 + k^2)u = 2\omega^2 k^2 u^3, \quad t \in [0, 1000],$$
$$u(0) = 0, \qquad u'(0) = 1$$

Table 3
$|z(t_n) - z_n|$, $\varepsilon = 0.001$, $t = 1000$

	Adaptive-NC			Adaptive-SC			Cowell			Adams		
h	$\omega = 1$	$\omega = 2$	$\omega = 3$	$\omega = 1$	$\omega = 2$	$\omega = 3$	$\omega = 1$	$\omega = 2$	$\omega = 3$	$\omega = 1$	$\omega = 2$	$\omega = 3$
1/20	$4.176 \cdot 10^{-10}$	$1.038 \cdot 10^{-9}$	$4.171 \cdot 10^{-9}$	$6.517 \cdot 10^{-10}$	$6.311 \cdot 10^{-9}$	$2.192 \cdot 10^{-8}$	$2.895 \cdot 10^{-8}$	$3.778 \cdot 10^{-6}$	$6.503 \cdot 10^{-5}$	$1.517 \cdot 10^{-6}$	$1.942 \cdot 10^{-4}$	$3.312 \cdot 10^{-3}$
1/10	$1.204 \cdot 10^{-10}$	$1.709 \cdot 10^{-8}$	$2.051 \cdot 10^{-7}$	$1.681 \cdot 10^{-9}$	$1.162 \cdot 10^{-7}$	$1.322 \cdot 10^{-6}$	$1.885 \cdot 10^{-6}$	$2.454 \cdot 10^{-4}$	$4.295 \cdot 10^{-3}$	$9.692 \cdot 10^{-5}$	$1.238 \cdot 10^{-2}$	$2.220 \cdot 10^{-1}$
1/5	$1.731 \cdot 10^{-8}$	$1.214 \cdot 10^{-6}$	$1.604 \cdot 10^{-5}$	$1.164 \cdot 10^{-7}$	$7.395 \cdot 10^{-6}$	$8.313 \cdot 10^{-5}$	$1.224 \cdot 10^{-4}$	$1.650 \cdot 10^{-2}$	$2.670 \cdot 10^{-1}$	$6.171 \cdot 10^{-3}$	$1.038 \cdot 10^{+0}$	$2.007 \cdot 10^{+5}$

Table 4
$|u(t_n) - u_n|$, $k = 0.1$, $t = 1000$

	Adaptive-NC			Adaptive-SC			Cowell			Adams		
h	$\omega = 1$	$\omega = 2$	$\omega = 3$	$\omega = 1$	$\omega = 2$	$\omega = 3$	$\omega = 1$	$\omega = 2$	$\omega = 3$	$\omega = 1$	$\omega = 2$	$\omega = 3$
1/20	$3.673 \cdot 10^{-11}$	$2.047 \cdot 10^{-10}$	$9.958 \cdot 10^{-10}$	$1.161 \cdot 10^{-10}$	$4.604 \cdot 10^{-9}$	$7.790 \cdot 10^{-9}$	$3.605 \cdot 10^{-9}$	$3.156 \cdot 10^{-7}$	$7.128 \cdot 10^{-6}$	$1.727 \cdot 10^{-7}$	$2.036 \cdot 10^{-5}$	$2.716 \cdot 10^{-4}$
1/10	$1.108 \cdot 10^{-10}$	$1.506 \cdot 10^{-8}$	$8.312 \cdot 10^{-8}$	$1.372 \cdot 10^{-9}$	$5.502 \cdot 10^{-8}$	$4.075 \cdot 10^{-7}$	$5.464 \cdot 10^{-7}$	$5.619 \cdot 10^{-5}$	$1.600 \cdot 10^{-3}$	$2.576 \cdot 10^{-5}$	$2.265 \cdot 10^{-3}$	$4.760 \cdot 10^{-1}$
1/5	$3.232 \cdot 10^{-8}$	$1.044 \cdot 10^{-6}$	$2.269 \cdot 10^{-6}$	$4.472 \cdot 10^{-7}$	$1.208 \cdot 10^{-6}$	$5.025 \cdot 10^{-5}$	$7.286 \cdot 10^{-5}$	$1.178 \cdot 10^{-2}$	$1.830 \cdot 10^{-1}$	$3.255 \cdot 10^{-3}$	$8.686 \cdot 10^{-1}$	$3.214 \cdot 10^{+0}$

with $\omega > 0$, $0 \leqslant k < \omega$. The analytic solution is

$$u(t) = \frac{1}{\omega}\,\mathrm{sn}(\omega t;\, k/\omega)$$

and represents a periodic motion in terms of an elliptic function. We have calculated the numerical solution in $t = 1000$, for the integration steps $h = \frac{1}{20}, \frac{1}{10}, \frac{1}{5}$, and parameter values $k = 0.1$ and $\omega = 1, 2, 3$. The absolute errors are tabulated (in $|\cdot|$-norm) in Table 4.

Example 3. We consider a nonintegrable dynamical system containing of two harmonic oscillators with equal frequencies in a perturbing field due to a polynomial potential (generalized Hénon–Heiles problem, see [1]) depending on two parameters. The study of this model problem is of great interest in quantum physics and in galactic dynamics. The model of perturbed Hamiltonian considered is

$$\mathscr{H} = \tfrac{1}{2}(X^2 + Y^2) + \tfrac{1}{2}\omega^2(x^2 + y^2) + \omega^2\alpha x^2 y - 2\omega^2\beta^2 y^4.$$

We use the initial conditions $Y = 0$, $x = 0$, $y = 0.5$ and $X = 0.5$ chosen in a neighbourhood of the origin since it retains the regular character of the orbits from the nonperturbed Hamiltonian. We select the parameter values $\omega = 1$, $\alpha = \beta = 0.01$ and integrate the problem with step size $h = 0.2$ for 5000 steps. In Fig. 1, the number of significative digits (sd) in error-propagation of the energy is shown, i.e.,

$$\mathrm{sd}(\mathscr{H}) = -\log_{10}(\max|\mathscr{H}_0 - \mathscr{H}_n|).$$

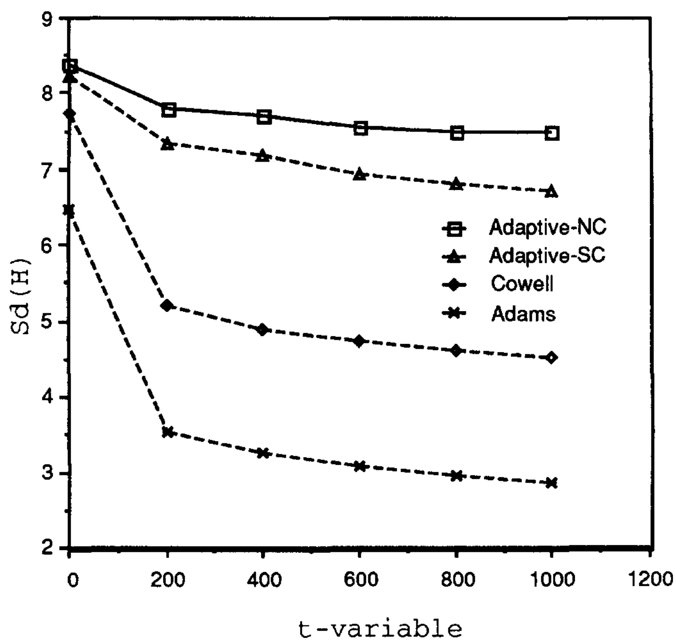

Fig. 1. Error-propagation of the energy.

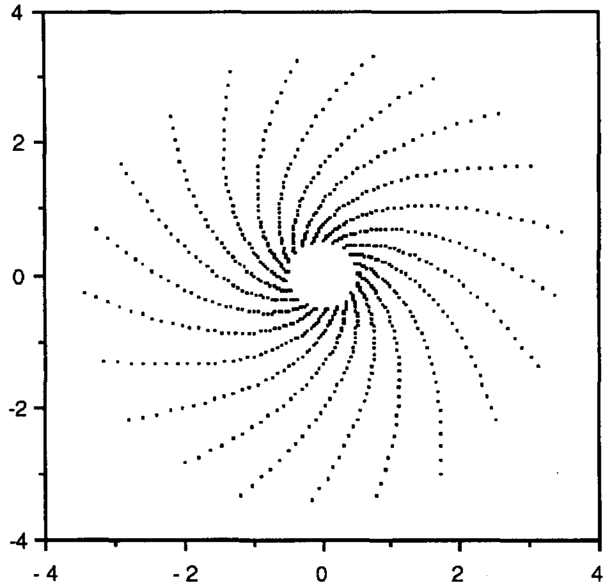

Fig. 2. Adams method ($h = 0.6$, $\alpha = 0.01$).

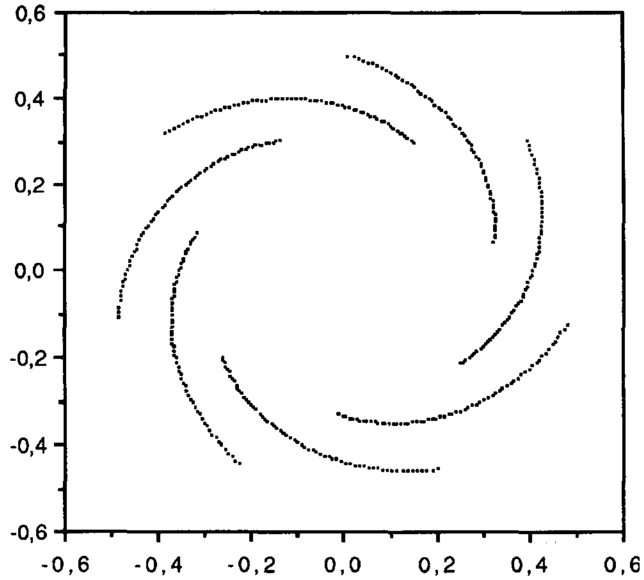

Fig. 3. Cowell method ($h = 0.9$, $\alpha = 0.01$).

In order to show the qualitative behaviour of the adaptive-NC methods with respect to classical constant coefficient methods (Adams and Cowell), we depict the x and y components of the solution using the parameter values $\omega = 1$, $\beta = \alpha$ for different values of α and time-steps. Figs. 2–4 correspond to perturbed problem with a small perturbation ($\alpha = 0.01$) and illustrate the orbital

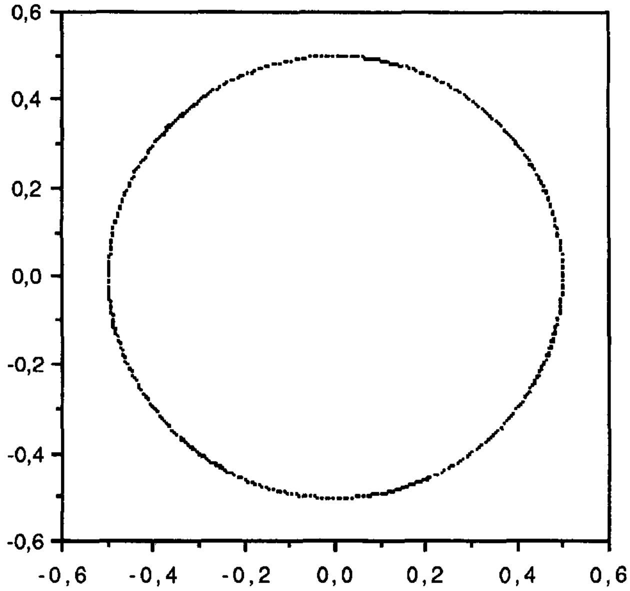

Fig. 4. Adaptive Nyström–Cowell method ($h = 0.9$, $\alpha = 0.01$).

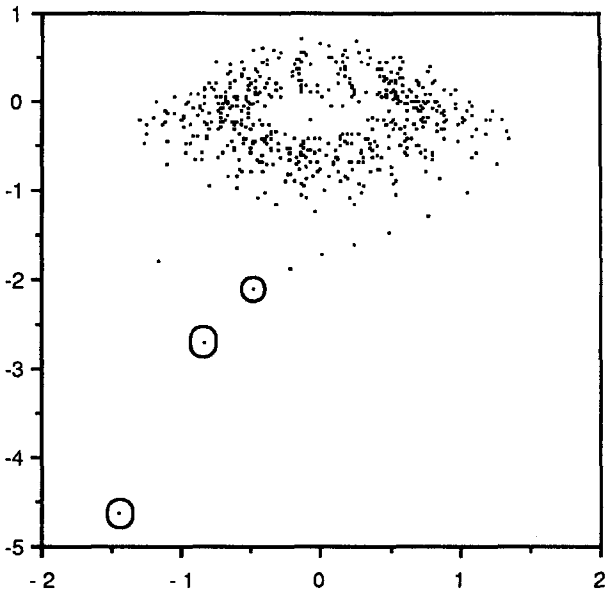

Fig. 5. Adams method ($h = 0.5$, $\alpha = 0.4$).

unstability of the Adams and Cowell methods for 500 steps versus the orbitally stable behaviour of the adaptive-NC methods. In Figs. 5–7 we depict the (x, y)-solution when the perturbation is comparable to unperturbed term ($\alpha = 0.4$) for 1000 steps, and the encircled points show as the numerical solution degenerates.

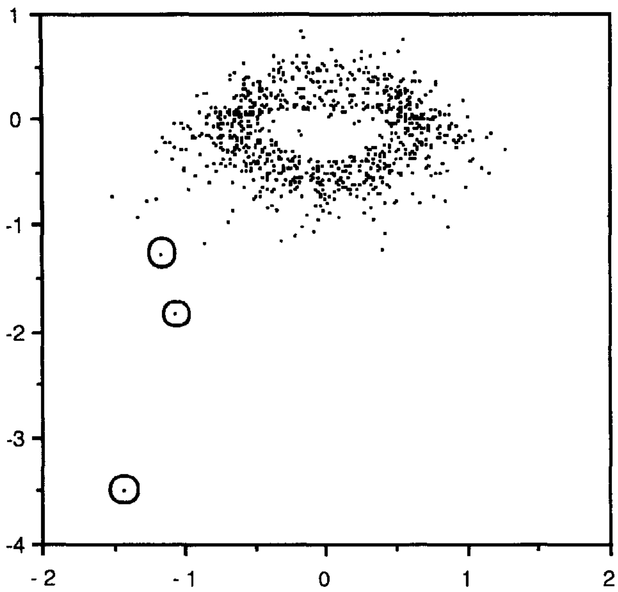

Fig. 6. Cowell method ($h = 0.9$, $\alpha = 0.04$).

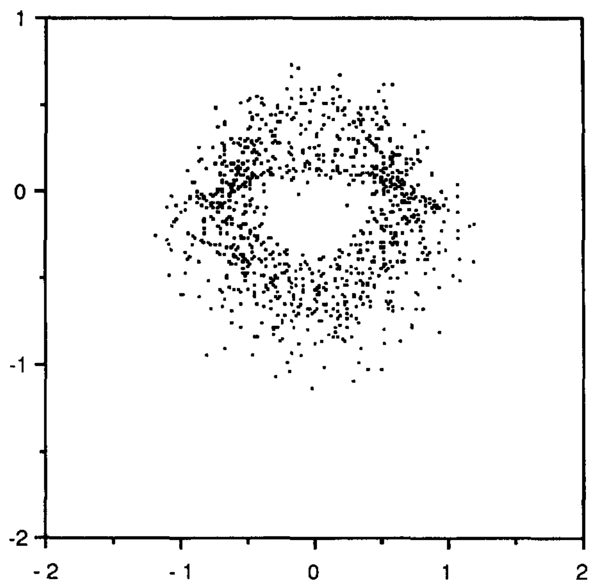

Fig. 7. Adaptive Nyström–Cowell method ($h = 0.9$, $\alpha = 0.4$).

5. Conclusions

From numerical results presented in Tables 3 and 4 and Figs. 1–7 we come to the following conclusions:

Adams methods yield poorer results than Cowell, adaptive-SC and adaptive-NC methods which are designed for second-order special equations of the form $y'' = f(t, y)$. In particular, Fig. 1 shows that the error-propagation degenerates much faster in the Adams methods.

Adaptive-NC methods are the most efficient for the test problems considered when the main frequency is known and the restoring terms represent a small perturbation. This result of better approximations by the adaptive-NC methods when compared with the adaptive-SC methods, is due to the fact that the error constants of the latter are bigger, although both types of methods have very similar properties of linear stability (orbital stability). In general, the error growth is much faster in the Adams and Cowell methods when the frequency ω increases, and at the end of the interval of integration the size of the error is approximately greater than three orders of magnitude with respect to the adaptive-NC methods.

The behaviour of orbital stability of the adaptive-NC method is shown in Fig. 4. This method yields the right qualitative behaviour of the solution circulating around the origin, whereas the Adams and Cowell methods spiral about it. Although the time-step considered for the Adams method is smaller, it degenerates very quickly. When the perturbation is not small ($\alpha = 0.4$), the solution computed by the adaptive-NC method circulates around the origin (see Fig. 7), but it degenerates very fast when it is obtained by the other methods (see the encircled points in Figs. 5 and 6). These algorithms fail in the 860th time-step approximately by reason of a numeric overflow. Of course, the nice appearance of Fig. 7 (which shows a good behaviour of the linear stability) when compared with Figs. 5 and 6 does not guarantee that the computed points are close to the corresponding values of the theoretical solution because the integration steps are very large. Undoubtedly, the adaptive-NC scheme have identified the right qualitative behaviour and this was the point of interest in these experiments.

The paper is limited to one positive eigenvalue; we intend to extend the method for the case of large second-order ODEs systems in the context of semidiscretized second-order hyperbolic equations. In these problems, there will appear a symmetric positive definite matrix (stiffness matrix) that contains implicitly the frequencies of the problem.

Acknowledgements

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Appendix. Error constants of the implicit adaptive NC and SC methods

In this appendix we present the local truncation error constants for the implicit Nyström–Cowell methods (denoted by $C_k^{\mathrm{N}}(v)$) and for the implicit Störmer–Cowell methods (denoted by $C_k^{\mathrm{S}}(v)$). In addition, for each order, we compare both error constants by means of the absolute value of the quotient between them, for typical values of v, i.e. v varying from 0 to 2.

(i) $k=4$ (Fig. 8)

Order of convergence:

- adaptive-NC: $p=6$,
- adaptive-SC: $p=5$.

Error constants:

$$C_5^{\mathrm{N}}(0) = -\tfrac{1}{1890}, \qquad C_4^{\mathrm{S}}(0) = -\tfrac{1}{240},$$

$$C_5^{\mathrm{N}}(v) = \frac{-90+165v^2-31v^4+(90+15v^2+v^4)\cos 2v}{90v^6(1-\cos 2v)}, \quad v \neq 0,$$

$$C_4^{\mathrm{S}}(v) = \frac{12-5v^2-(12+v^2)\cos v}{12v^4(1-\cos v)}, \quad v \neq 0.$$

(ii) $k=5$ (Fig. 9)

Orders of convergence:

- adaptive-NC: $p=6$,
- adaptive-SC: $p=6$.

Error constants:

$$C_5^{\mathrm{N}}(0) = -\tfrac{1}{1890}, \qquad C_5^{\mathrm{S}}(0) = -\tfrac{221}{60480},$$

$$C_5^{\mathrm{N}}(v) = \frac{-90+165v^2-31v^4+(90+15v^2+v^4)\cos 2v}{90v^6(1-\cos 2v)}, \quad v \neq 0,$$

$$C_5^{\mathrm{S}}(v) = \frac{-360+480v^2-139v^4+(360-300v^2-26v^4)\cos v}{360v^6(1-\cos v)}, \quad v \neq 0.$$

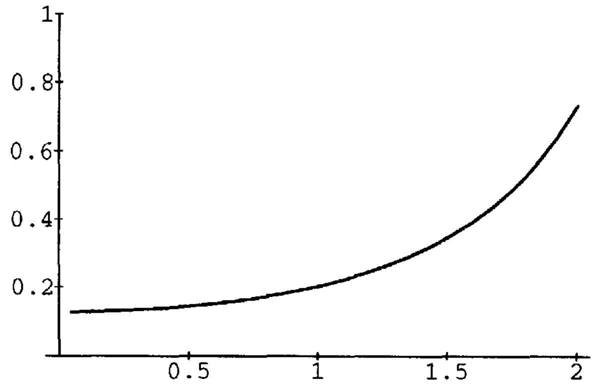

Fig. 8. $|C_5^N(v)/C_5^S(v)|$ for $v \in [0,2]$.

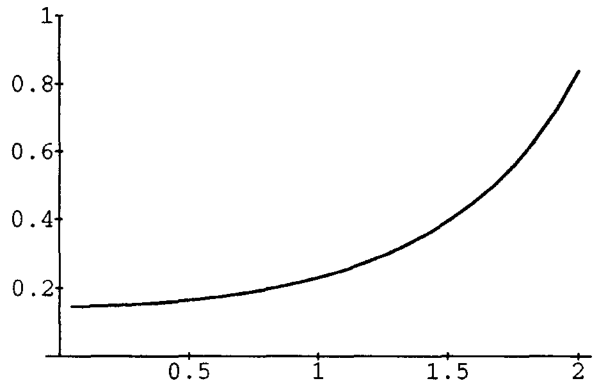

Fig. 9. $|C_5^N(v)/C_4^S(v)|$ for $v \in [0,2]$.

(iii) $k = 6$ (Fig. 10)

Order of convergence:

- adaptive-NC: $p = 7$,
- adaptive-SC: $p = 7$.

Error constants:

$$C_6^N(0) = -\tfrac{1}{1890}, \qquad C_6^S(0) = -\tfrac{19}{6048},$$

$$C_6^N(v) = \frac{-90 + 165v^2 - 31v^4 + (90 + 15v^2 + v^4)\cos 2v}{90v^6(1 - \cos 2v)}, \quad v \neq 0,$$

$$C_6^S(v) = \frac{-360 + 300v^2 - 64v^4 + (360 - 120v^2 - 11v^4)\cos v}{180v^6(1 - \cos v)}, \quad v \neq 0.$$

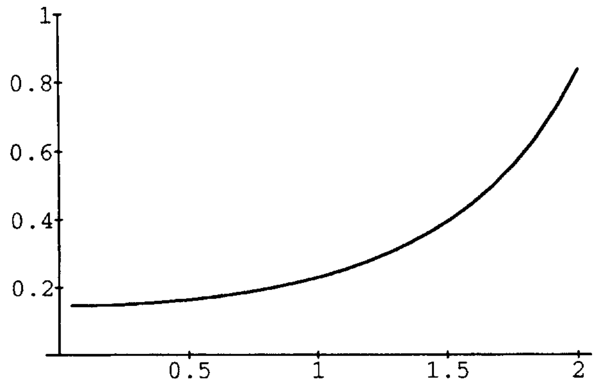

Fig. 10. $|C_6^{\mathrm{N}}(v)/C_6^{\mathrm{S}}(v)|$ for $v \in [0,2]$.

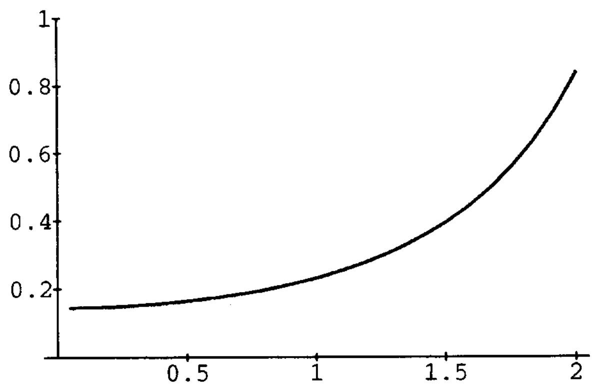

Fig. 11. $|C_7^{\mathrm{N}}(v)/C_7^{\mathrm{S}}(v)|$ for $v \in [0,2]$.

(iv) $k = 7$ (Fig. 11)
Order of convergence:

- adaptive-NC: $p = 8$,
- adaptive-SC: $p = 8$.

Error constants:

$$C_7^{\mathrm{N}}(0) = -\tfrac{109}{226\,800}, \qquad C_7^{\mathrm{S}}(0) = -\tfrac{9829}{3\,628\,800},$$

$$C_7^{\mathrm{N}}(v) = \frac{5040 - 13860v^2 + 10227v^4 - 1629v^6}{5040v^8(1-\cos 2v)} + \frac{(-5040 + 3780v^2 + 693v^4 + 47v^6)\cos 2v}{5040v^8(1-\cos 2v)}, \quad v \neq 0,$$

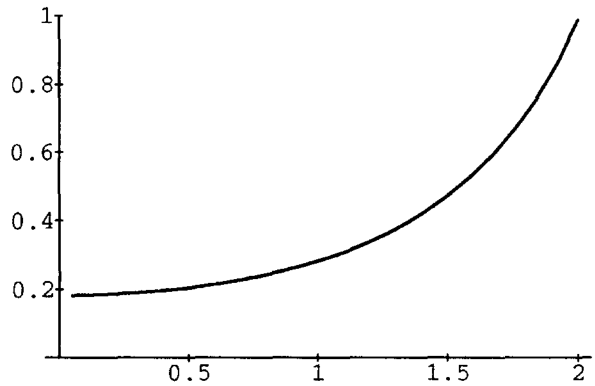

Fig. 12. $|C_8^{\mathrm{N}}(v)/C_8^{\mathrm{S}}(v)|$ for $v \in [0,2]$.

$$C_7^{\mathrm{S}}(v) = \frac{5040 - 16380v^2 + 9807v^4 - 1657v^6}{5040v^8(1-\cos v)} + \frac{(-5040 + 13860v^2 - 2667v^4 - 261v^6)\cos v}{5040v^8(1-\cos v)}, \quad v \neq 0$$

(v) $k = 8$ (Fig. 12)

Order of convergence:

- adaptive-NC: $p = 9$,
- adaptive-SC: $p = 9$.

Error constants:

$$C_8^{\mathrm{N}}(0) = -\tfrac{7}{16200}, \qquad C_8^{\mathrm{S}}(0) = -\tfrac{407}{172\,800},$$

$$C_8^{\mathrm{N}}(v) = \frac{5040 - 11340v^2 + 5607v^4 - 761v^6}{2520v^8(1-\cos 2v)} + \frac{(-5040 + 1260v^2 + 273v^4 + 19v^6)\cos 2v}{2520v^8(1-\cos 2v)}, \quad v \neq 0,$$

$$C_8^{\mathrm{S}}(v) = \frac{15120 - 23940v^2 + 10941v^4 - 1541v^6}{5040v^8(1-\cos v)} - \frac{(-15120 - 16380v^2 + 2121v^4 + 233v^6)\cos v}{5040v^8(1-\cos v)}, \quad v \neq 0.$$